

Orbital physics of polar Fermi molecules

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We study a system of polar dipolar fermions in a two-dimensional optical lattice and show that multi-band Fermi-Hubbard model is necessary to discuss such system. By taking into account both on-site, and long-range interactions between different bands, as well as occupation-dependent inter- and intra-band tunneling, we predict appearance of novel phases in the strongly-interacting limit.

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Creation of ultracold hetero-nuclear molecules opens the path towards experimental realization of strongly-interacting dipolar many-body systems. Depending on the constituent atoms, in moderate electric field these molecules can have large dipole moment of 1 Debye in their vibrational ground states [1–4]. In particular, fermionic molecules in presence of an optical lattice can be used to simulate various quantum phases, such as quantum magnetism and phases of t – J like models [5, 6], various charge density wave orders [7, 8], bond-order solids [9] etc. One should also stress that in the strongly correlated regime, both in bosonic and fermionic systems the standard descriptions of single-band Hubbard model ceases to be valid. The effect of higher bands become important leading to novel phases like pair-superfluidity etc [10–15].

While most of the works have dealing with higher bands concentrated on bosonic systems, in this paper, we study dipolar fermions confined in 2D optical lattice $V_{\text{latt}} = V_0 [\sin^2(\pi x/a) + \sin^2(\pi y/a)] + \frac{m\Omega^2}{2}z^2$, where V_0 is the lattice depth, a is the lattice constant, m is the mass of the molecule, and Ω is the frequency of harmonic potential in z direction. The dipoles are polarized along the direction of harmonic trapping. Usually, at low temperature and for low tunneling, the phase diagram consists of different crystal states whose structure depends on the filling n [7]. In this paper, we derive a Fermi-Hubbard model for dipolar fermions including the effects of higher bands. We show that, even for moderate dipolar strength, it is necessary to take into account the excitations along the z direction. Simultaneously, in this regime, the interaction induced hoppings along the lattice give also important contributions. This changes the phases expected for a spinless Hubbard model including only a single band. Near $n \gtrsim 1/4$, we find a crossover to one dimensional (1D) chains of decoupled Luttinger liquids along with density wave order. Near $n \gtrsim 1/2$, we find that the system can be mapped to an extended pseudo-spin 1/2 Hubbard model with different emergent lattice configuration. We find a regime where chiral p -wave superconductivity emerges through Kohn-Luttinger mechanism with transition temperature T_c of the order

of tunneling. This gives rise to an exotic supersolid, with the diagonal long-range order provided by the checker-board pattern of the lower orbital fermions, while the superfluidity originating from the fermions in the higher band.

The Hamiltonian for the dipolar fermions in the second quantized form reads $H = \int d^3\mathbf{r} \Psi^\dagger(\mathbf{r}) H_0 \Psi(\mathbf{r}) + \frac{1}{2} \int d^3\mathbf{r} d^3\mathbf{r}' \Psi^\dagger(\mathbf{r}) \Psi^\dagger(\mathbf{r}') \mathcal{V}(\mathbf{r} - \mathbf{r}') \Psi(\mathbf{r}') \Psi(\mathbf{r})$, where $\Psi(\mathbf{r})$ is a spinless fermion field operator. In the units of recoil energy $E_R = \pi^2 \hbar^2 / (2ma^2)$, the single particle Hamiltonian becomes $H_0 = -\nabla^2 + V_{\text{latt}}(\mathbf{r})/E_R$ and the long-range interaction potential $\mathcal{V}(\mathbf{r}) = D(1/r^3 - 3z^2/r^5)$, where $D = 2\pi m d^2 / (\hbar^2 a)$ is a dimensionless dipolar strength, related to the electric dipolar moment d . For KRb molecules with a dipole moment of 0.5 Debye confined in the optical lattice with $a = 345\text{nm}$ [16] one gets $D = 8.6$. We decompose the field operator in the basis of Wannier functions in the x, y directions and of harmonic oscillator eigenstates in z direction. For convenience we introduce orbital index $\sigma = \{pml\}$ denoting p, m and l excitations in x, y , and z direction respectively. In this basis the field operator $\Psi(\mathbf{r}) = \sum_{\mathbf{i}, \sigma} \hat{a}_{\mathbf{i}\sigma} \mathcal{W}_{\mathbf{i}\sigma}(\mathbf{r})$, where $\mathcal{W}_{\mathbf{i}\sigma}(\mathbf{r})$ is the single-particle wave-function in orbital σ localized on site $\mathbf{i} = i_x \mathbf{e}_x + i_y \mathbf{e}_y$ (\mathbf{e}_x and \mathbf{e}_y are unit vectors in the proper directions). Fermionic operator $\hat{a}_{\mathbf{i}\sigma}$ annihilates particle in this state. The Hamiltonian can be rewritten in the following Hubbard-like form $H = \sum_{\sigma} \mathcal{H}_{\sigma}^{(1)} + \sum_{\sigma\sigma'} \mathcal{H}_{\sigma\sigma'}^{(2)}$, where

$$\mathcal{H}_{\sigma}^{(1)} = E_{\sigma} \sum_{\mathbf{i}} \hat{n}_{\mathbf{i}\sigma} + J_{\sigma} \sum_{\{\mathbf{i}\mathbf{j}\}} \hat{a}_{\mathbf{i}\sigma}^{\dagger} \hat{a}_{\mathbf{j}\sigma} \quad (1a)$$

$$\begin{aligned} \mathcal{H}_{\sigma\sigma'}^{(2)} = & U_{\sigma\sigma'} \sum_{\mathbf{i}} \hat{n}_{\mathbf{i}\sigma} \hat{n}_{\mathbf{i}\sigma'} + \sum_{\mathbf{i} \neq \mathbf{j}} V_{\sigma\sigma'}(\mathbf{i} - \mathbf{j}) \hat{n}_{\mathbf{i}\sigma} \hat{n}_{\mathbf{j}\sigma} \\ & + \sum_{\{\mathbf{i}\mathbf{j}\}} \sum_{\sigma''} T_{\sigma\sigma'}^{\sigma''}(\mathbf{i} - \mathbf{j}) \hat{a}_{\mathbf{i}\sigma}^{\dagger} \hat{n}_{\mathbf{i}\sigma''} \hat{a}_{\mathbf{j}\sigma'}. \end{aligned} \quad (1b)$$

Parameters E_{σ} and J_{σ} comes from the single particle Hamiltonian and denote single-particle energy and nearest-neighbour tunneling in orbital σ respectively. The inter-particle interaction has three contributions to the Hamiltonian (1b): (i) the on-site interaction energy of fermions occupying different orbitals σ and σ' of the

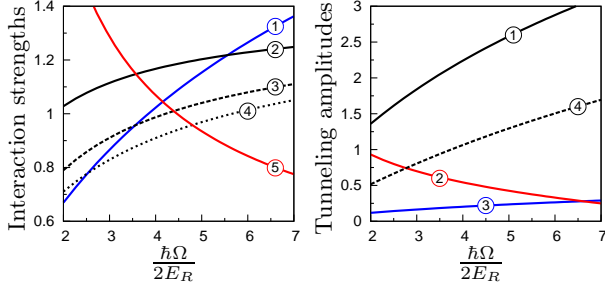


FIG. 1. Parameters of the Hamiltonian for $V_0 = 8E_R$ as functions of the lattice confinement. (a) On-site interaction $-\frac{U_{s,p_z}}{DE_R}$ (blue solid line -1-), and nearest-neighbor long-range interactions $\frac{V_{s,s}(e_x)}{DJ_s}$ (solid black line -2-), $\frac{V_{s,p_z}(e_x)}{DJ_s}$ (dashed black line -3-), and $\frac{V_{p_z,p_z}(e_x)}{DJ_s}$ (dotted black line -4-). The red line -5- shows the ratio $V_{p_z,p_z}(2e_x)/T_{\text{eff}}^{\parallel}$. (b) Magnitudes of the induced tunneling terms $\frac{T_{p_z,p_z}^s(e_x)}{DJ_s}$ (black solid line -1-), $\frac{T_{s,p_z}^s(e_x)}{DJ_s}$ (red solid line -2-), and $\frac{T_{p_z,p_z}^s(e_x)}{DJ_s}$ (blue solid line -3-). The dashed black line -4- denotes the ratio $T_{\text{eff}}^{\parallel}/J_s$ for $D = 10$.

same site $U_{\sigma\sigma'}$, (ii) the long-range interaction energy of fermions occupying orbitals σ and σ' of different sites $V_{\sigma\sigma'}(\mathbf{i} - \mathbf{j})$, (iii) and the tunneling from orbital σ' at site \mathbf{j} to the orbital σ at site \mathbf{i} induced by presence of an additional fermion at site \mathbf{i} in orbital σ'' denoted by $T_{\sigma\sigma'}^{\sigma''}(\mathbf{i} - \mathbf{j})$.

The Hamiltonian (1) is very general. To get a physical understanding of its properties, we start by examining the properties of density-density interactions. We calculate the interactions between few lowest bands: $s = \{000\}$, $p_x = \{100\}$, $p_y = \{010\}$, $p_z = \{001\}$, $p_{xz} = \{101\}$, and $p_{yz} = \{011\}$. We find that the on-site interactions $U_{s,p_x} = U_{s,p_y}$ is always repulsive. It means that putting two fermions in s and p_x or p_y band simultaneously is energetically unfavorable. Remarkably we find that U_{s,p_z} is always negative. This surprising attraction stems from the presence of the fermionic exchange term and the shape of the dipolar interactions (see supplementary material). Moreover, as it is seen from Fig. 1a, this interaction can not be neglected even for stronger confinements in z directions. For higher orbitals we find that $U_{s,p_z} \ll U_{s,p_{xz}} = U_{s,p_{yz}} < 0$. In addition for long-range interactions we find that $V_{s,s}(\mathbf{i}) > V_{s,p_z}(\mathbf{i}) > V_{p_z,p_z}(\mathbf{i}) > 0$. From this analysis we conclude that for polar molecules there always exists some critical dipolar strength for which single-band approximation breaks down since two particles can occupy the same site. This critical behavior is controlled by the on-site energy cost $\Delta = E_{p_z} + U_{s,p_z}$. In this paper we consider situations when Δ is positive.

Next we discuss the role of the interaction induced tunnelings in Hamiltonian (1). Counter intuitively the

most important contribution does not come from the induced tunneling in p_z band (T_{p_z,p_z}^s), but from the inter-band tunneling which changes p_z orbital to the p_{xz} and p_{yz} ones ($T_{p_z,p_{xz}}^s(e_x)$). Note, that this inter-band tunneling is absent for usual single-particle tunneling due to the properties of single particle Hamiltonian [19]. From properties of p orbital states it follows that $T_{p_z,p_{xz}}^s(-e_x) = -T_{p_z,p_{xz}}^s(e_x)$. The relation of this term to other interaction-induced tunnelings is shown in Fig. 1b. From the above analysis we introduce simplified, but realistic model of polar Fermi molecules confined in 2D optical lattice by taking into account effects of interactions between orbitals $\sigma \in \{s, p_z, p_{xz}, p_{yz}\}$.

Since we consider the case when $\Delta > 0$, therefore for low filling all fermions occupy only the s orbital states. For filling $n = 1/4$ and large enough D ($\gtrsim 3$) there is non vanishing single-particle excitation gap and the system is in the s -band insulator state (denoted by blue spheres in Fig. 2a) [7]. Situation change dramatically for higher fillings. It can be simply understood with energy arguments. The energy cost of putting additional particle in the vacant site is given by $E_{\text{vac}} = V_{s,s}(e_x) + 2V_{s,s}(e_x + e_y) + \dots$. In contrast the cost of putting additional particle to the p_z orbital of an occupied site $E_{\text{occ}} = \Delta + 2V_{s,p_z}(2e_x) + \dots$. For D larger than some critical strength one finds that $E_{\text{occ}} < E_{\text{vac}}$. As an example, such conditions are fulfilled for $V_0 = 8E_R$, $D = 10$, and $\hbar\Omega \leq 14E_R$. Consequently, additional particles start to fill p_z band of previously occupied sites. In this scenario energy conserving dynamics of the system comes from the second-order processes involving tunneling to the next occupied site (along x direction in Fig. 2a). To the leading order, this effective tunneling is given by

$$T_{\text{eff}}^{\parallel} \approx T_{s,p_z}^s(e_x)^2 / (|U_{s,p_z}| + E_{p_{xz}} - E_{p_z}). \quad (2)$$

Thus, the p_z fermions will only move along one direction chosen by the insulator checkerboard geometry in s -band. The resulting system can be thought as stacks of independent, one-dimensional chains without inter-chain tunnelings. Each chain is characterized by the effective tunneling $T_{\text{eff}}^{\parallel}$ and the nearest-neighbor interaction $V_{p_z,p_z}(2e_x)$. Relation between these parameters can be tuned experimentally by changing the trap confinement (red line -5- in Fig. 1a) as well as the lattice depth. Moreover, due to the absence of the inter-chain tunnelings, we can apply Jordan-Wigner transformation to each chain to map it to chain of independent spin 1/2 XXZ model resulting in a crossover to one-dimensional system. For $2T_{\text{eff}}^{\parallel} > V_{p_z,p_z}(2e_x)$ such a model will show metallic behaviour with the low energy sector is dominated by the bosonic excitations. From Fig. 1 we see that indeed $V_{p_z,p_z}(2e_x)/T_{\text{eff}}^{\parallel} < 2$ for any confinement for $V_0 = 8E_R$ and $D = 10$. Thus we will see metallic behaviour of the system due p_z fermions with the s orbital fermions form-

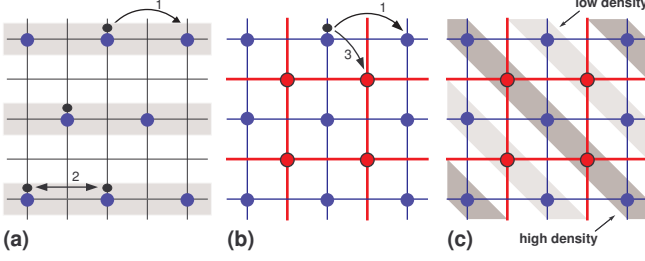


FIG. 2. Pictorial diagram of the different checker board lattices. The blue and shaded-red sphere denotes s -orbital fermions and the smaller black sphere denotes p_z orbital fermions. (a) Checkerboard lattice at $n = 1/4$ filling. The p_z fermions will move with effective tunneling $T_{\text{eff}}^{\parallel}$ (arrow 1) only along the shaded region making a stack of 1D chains. Interaction between neighboring p -band fermions is equal to $V_{p_z, p_z}(2\mathbf{e}_x)$ (arrow 3). (b) Checkerboard lattice at $n = 1/2$. The blue and thick-red line constitutes two different sub-lattices which are not connected via tunneling processes since the tunneling T_{eff}^{\perp} (arrow 2) is much smaller than $T_{\text{eff}}^{\parallel}$. (c) Density-wave structure at filling $\delta n = 1/4$. The dark and light shadings denote higher and lower density of the p_z fermions respectively.

ing a checkerboard density pattern as shown in Fig. 2a.

Next let us discuss the case of filling $n = 1/2$. Then for low dipolar strength D , due to the same reasons as before fermions will occupy only the s -band. To look into properties of the ground state, we express the average density $\langle \hat{n}_{i,s} \rangle = (1 + (-1)^{i_x + i_y} \delta)/2$, where δ is the order parameter. We also define the single-particle imaginary time Green functions $\mathcal{G}(\mathbf{i} - \mathbf{j}, \tau) = \langle \mathcal{T} \hat{a}_{i,s}(\tau) \hat{a}_{j,s}^\dagger(0) \rangle$. By following the procedure described in [17, 18] we find the following equations for \mathcal{G} in the momentum space

$$[\omega + \mu - 2V(1 - \delta')] G_1(\mathbf{k}, \omega) - \epsilon_{\mathbf{k}} G_2(\mathbf{k}, \omega) = 1, \quad (3a)$$

$$[\omega + \mu - 2V(1 + \delta')] G_2(\mathbf{k}, \omega) - \epsilon_{\mathbf{k}} G_1(\mathbf{k}, \omega) = 0, \quad (3b)$$

where in the position space $G_1(\mathbf{i})$ ($G_2(\mathbf{i})$) is equal to $\mathcal{G}(\mathbf{i})$ for $i_x + i_y$ even (odd). The kinetic energy $\epsilon_{\mathbf{k}} = 2J_s(\cos k_x a + \cos k_y a)$, the effective potential $V = \sum_{\mathbf{i} \neq 0} V_{ss}(\mathbf{i})$, and $\delta' = \delta(\sum_{\mathbf{i} \in \text{odd}} V_{ss}(\mathbf{i}) - \sum_{\mathbf{i} \in \text{even}} V_{ss}(\mathbf{i}))/V$. These mean field equations for G_1 and G_2 are similar to the ones found for extended Hubbard model, with a renormalized nearest neighbour interaction and density imbalance [17, 18]. In our case we consider the neighbors within a radius of $|\mathbf{i}| \leq 5$. Then, by solving equations (3), we find that in the strong coupling limit $\delta = 1 - \frac{3J_s^2}{2V_{ss}^2(\mathbf{e}_x)}$ ($\delta \sim .98$ for previous parameters). Thus, we find that in this limit the ground state of the system is the checkerboard insulator (blue and thick-red spheres in Fig. 2b).

Next we look to properties of the system with additional particles. To do it we define deviation from half-filling $\delta n = n - 1/2$ and we introduce corresponding chemical potential $\mu(\delta n)$. From energy arguments

we find that two scenario can happen. The additional fermion (i) occupies a vacant site with energy cost $E_{\text{vac}} = 4V_{s,s}(\mathbf{e}_x) + 8V_{s,s}(2\mathbf{e}_x + \mathbf{e}_y) + \dots$ or (ii) it goes to the p_z orbital of an occupied site with energy cost $E_{\text{occ}} = \Delta + 4V_{s,p_z}(\mathbf{e}_x + \mathbf{e}_y) + V_{s,p_z}(2\mathbf{e}_x) + \dots$. Consequently, in the second scenario (when $E_{\text{occ}} \leq E_{\text{vac}}$), all extra fermions will occupy the p_z orbitals of the already occupied sites. As an example, such conditions are fulfilled for $V_0 = 8E_R$, $D = 8$, and $\hbar\Omega \leq 10E_R$. In such a case δn corresponds to the filling of p_z band fermions. The parallel tunneling of the p_z fermions between the occupied sites will again arise from the second order processes (2). Moreover, tunneling to the diagonally occupied site $T_{\text{eff}}^{\perp} \approx -[J_s - T_{p_z, p_z}^s(\mathbf{e}_x)]^2 / |U_{s, p_z}|$ for $D \sim 10$ it is 400 smaller than $T_{\text{eff}}^{\parallel}$. Consequently fermions in the p_z orbitals can move in independent square sub-lattices (either the thick-red or blue sub-lattice shown in the Fig. 2b). Note, that fermions can not tunnel between different sub-lattices. Thus we can describe the system of the p_z fermions in the blue (thick-red) lattice as pseudo-spin up (down). By introducing operators $\hat{c}_{i,s}$, where $s \in \{\uparrow, \downarrow\}$ the effective Hamiltonian can be written as $H_{\text{eff}} = T_{\text{eff}}^{\parallel} \sum_s \sum_{\{ij\}} \hat{c}_{i,s}^\dagger \hat{c}_{j,s} + H_{\text{int}}$ with

$$H_{\text{int}} = V_{\uparrow\uparrow} \sum_s \sum_{\{ij\}} \hat{n}_{i,s} \hat{n}_{j,s} + V_{\uparrow\downarrow} \sum_{[ij]} \hat{n}_{i\uparrow} \hat{n}_{j\downarrow}, \quad (4)$$

where $\hat{n}_{i,s} = \hat{c}_{i,s}^\dagger \hat{c}_{i,s}$. For convenience we introduce $V_{\uparrow\uparrow} = V_{p_z, p_z}(2\mathbf{e}_x)$ and $V_{\uparrow\downarrow} = V_{p_z, p_z}(\mathbf{e}_x + \mathbf{e}_y)$. Note, that now $\{.\}$ is understood as a nearest-neighbor in a given sub-lattice. Nearest-neighbors between different sub-lattices is denoted by $[.]$. The modified lattice constant of the sub-lattices is $\tilde{a} = 2a$. In this way we are able to investigate the system properties with weak-coupling theory. To do this we transform to momentum space and introduce charge fluctuations $\rho_{\mathbf{q}} = \sum_{\mathbf{k}, s} c_{\mathbf{k}+\mathbf{q}, s}^\dagger c_{\mathbf{k}, s}$ and spin fluctuations $S_{\mathbf{q}} = \sum_{\mathbf{k}, s} s c_{\mathbf{k}+\mathbf{q}, s}^\dagger c_{\mathbf{k}, s}$ operators. Subsequently we write

$$H_{\text{int}} = \frac{1}{4} \sum_{\mathbf{q}} (2V_{\uparrow\uparrow} \eta_{\mathbf{q}} + V_{\uparrow\downarrow} \beta_{\mathbf{q}}) \rho_{\mathbf{q}} \rho_{-\mathbf{q}} + \frac{1}{4} \sum_{\mathbf{q}} (2V_{\uparrow\uparrow} \eta_{\mathbf{q}} - V_{\uparrow\downarrow} \beta_{\mathbf{q}}) S_{\mathbf{q}} S_{-\mathbf{q}}, \quad (5)$$

where $\eta_{\mathbf{q}} = 2(\cos(q_x \tilde{a}) + \cos(q_y \tilde{a}))$ and $\beta_{\mathbf{q}} = 4(\cos(q_x \tilde{a}/2) \cos(q_y \tilde{a}/2))$. The system with interactions described by (5) can manifest three possible magnetic instabilities: charge-density wave (CDW), spin-density wave (SDW), and ferromagnetic instability. At $\delta n = 1/4$ (each sub-lattice is half-filled in p orbital), as $\beta_{\mathbf{q}} = 0$ for nesting vector $\mathbf{q} \tilde{a} = (\pm\pi, \pm\pi)$, interaction in the spin channel becomes repulsive and therefore SDW order is absent. We also find that Stoner ferromagnetism occurs only for very low temperature on the order of $10^{-4} \times T_{\text{eff}}^{\parallel}$ and therefore it can hardly be observed.

Finally, we examine the CDW instability at $\delta n = 1/4$ with modulation $\mathbf{q}\tilde{a} = (\pm\pi, \pm\pi)$. Within weak coupling theory, the transition temperature of the CDW state for the system described by the Hamiltonian (4) is given by $T_{\text{CDW}} \approx 8T_{\text{eff}}^{\parallel} \exp\left(-\pi\sqrt{T_{\text{eff}}^{\parallel}/V_{\uparrow\uparrow}}\right)$. It means that transition temperature is of the same order as tunneling energy in the s -band. For example, when $V_0 = 8E_R$, $\hbar\Omega = 10E_R$, and $D = 8$ we find that $T_{\text{CDW}} \approx 0.35J_s$ (~ 2 nK). One should note that due to the relative shift of sub-lattices the resulting density modulation in this phase looks like stripes rather than standard checkerboard structure as shown in Fig. 2c.

Lastly, we investigate the emergence of triplet superconductivity between the same pseudo-spin fermions, arising via Kohn-Luttinger mechanism (KL) [19]. We look for Cooper pairs with chiral p -wave symmetry. The effective interaction between fermions in KL mechanism in terms of the scattering momentum $\mathbf{k} - \mathbf{k}' = \mathbf{q}$ can be written as

$$V_{\text{eff } s,s}(\mathbf{q}) = V_{\uparrow\uparrow}\eta_{\mathbf{q}} - \sum_{\mathbf{p}} \left[(V_{\uparrow\uparrow}^2\eta_{\mathbf{q}}^2 + V_{\uparrow\downarrow}^2\beta_{\mathbf{q}}^2) Q_{\mathbf{q},\mathbf{p}} - 2V_{\uparrow\uparrow}^2\eta_{\mathbf{q}}\eta_{\mathbf{k}-\mathbf{p}}Q_{\mathbf{q},\mathbf{p}} - V_{\uparrow\uparrow}^2\eta_{\mathbf{k}'-\mathbf{p}}\eta_{\mathbf{k}-\mathbf{p}}Q_{\mathbf{k}+\mathbf{k}',\mathbf{p}} \right], \quad (6)$$

where $Q_{\mathbf{q},\mathbf{p}} = \frac{f(\epsilon_{\mathbf{p}}) - f(\epsilon_{\mathbf{p}-\mathbf{q}})}{\epsilon_{\mathbf{p}-\mathbf{q}} - \epsilon_{\mathbf{p}}}$, $f(\epsilon)$ is the Fermi distribution function and $\epsilon_{\mathbf{p}} = 2T_{\text{eff}}^{\perp}(\cos(q_x\tilde{a}) + \cos(q_y\tilde{a}))$ is the dispersion. The summation in (S3) comes from taking into account the second-order terms represented by diagrams shown in Fig. 3a. By performing the integration over the momentum in the limit of $T \rightarrow 0$, we finally get antisymmetric part of effective coupling $\{V_{\text{eff}}(\mathbf{q})\}_- = -\lambda(T, \mu)(\sin(k_x\tilde{a})\sin(k'_x\tilde{a}) + \sin(k_y\tilde{a})\sin(k'_y\tilde{a}))$ where $\lambda(T, \mu) = 2V_{\uparrow\uparrow} + \frac{V_{\uparrow\uparrow}^2}{\pi T_{\text{eff}}}F_1(T, \mu) - \frac{V_{\uparrow\uparrow}^2}{\pi T_{\text{eff}}}F_2(T, \mu)$. Functions F_1 and F_2 originate in the second-order corrections and their detailed forms are given in the supplementary material. The point is that, due to the Van-Hove singularity in density of states, function F_2 contains a logarithmic divergence. At the same time function F_1 is analytical due to the dressing of the density of states. This means that there always exists finite critical μ above which the interaction is attractive and superfluidity appears. From the BCS theory one can get an estimate of the transition temperature T_c (derivation is shown in Supplementary material). In Fig. 3b we plot the transition temperature T_c as a function of deviation δn for example parameters discussed previously. For $\delta n \sim 0.22$ we get $T_c \sim 0.2J_s$ (~ 1 nK). At half-filling with $\delta n = 1/4$ for the red and blue lattices, the transition temperatures for the CDW and superfluidity are similar. This will result in a competition between both instabilities. A detailed account of such scenario is beyond this scope of this paper.

In conclusion, we have derived a generalized Hubbard model for dipolar fermions in an optical lattice by tak-

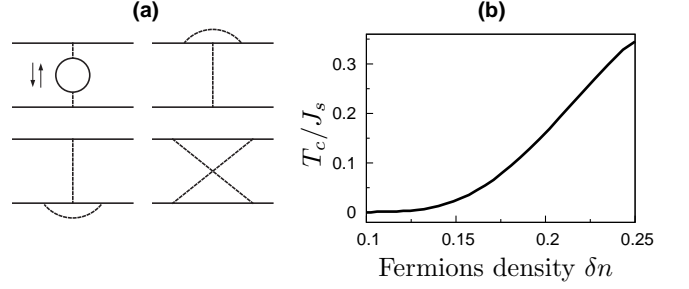


FIG. 3. (a) Diagrammatic representation of the second order contributions in (S3). (b) p -wave superfluid transition temperature T_c as a function of density $n = 1/2 + \delta n$.

ing into account higher orbitals. We have shown that the effect of these higher orbitals leads to new phenomena. Due to the strong interaction-dependent hopping terms in higher orbitals, these systems can be described by effective weakly-interacting theories. For particular parameters, near $n \gtrsim 1/4$, we found a cross-over to the one-dimensional physics resulting in simultaneous metallic and density wave properties. For other set of parameters, $n \gtrsim 1/2$, the system can be described by a weakly interacting Hubbard model with pseudo-spin originating from the lattice geometry. Using the Kohn-Luttinger theory, we found a transition to the chiral p -wave superfluidity without destroying the checkerboard order. The parameters used here are currently experimentally achievable.

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- [1] K. Ni, et. al., Science **322**, 231 (2008).
 - [2] J. Deiglmayr, et. al., Faraday Discuss. **142**, 335 (2009).
 - [3] M. Debatin, et. al., arXiv:1106.0129.
 - [4] J. W. Park, et. al., arXiv:1110.4552.
 - [5] A. V. Gorshkov, et. al., Phys. Rev. Lett. **107**, 115301 (2011).
 - [6] K. A. Kuns, A. M. Rey, and A. V. Gorshkov, Phys. Rev. A **84**, 063639 (2011).
 - [7] K. Mielsonson, and J. K. Freericks, Phys. Rev. A **83**, 043609 (2011).
 - [8] A.-L. Gadsbølle and G. M. Bruun arxiv: 1112.2846.
 - [9] S. G. Bhongale, et. al. arxiv: 1111.2873.
 - [10] D. -S. Luehmann, O. Juergensen, and K. Sengstock, arXiv:1108.3013.
 - [11] A. Mering, and M. Fleischhauer, Phys. Rev. A, **83**, 063630 (2011).
 - [12] U. Bissbort, F. Deuretzbacher, and W. Hofstetter, arXiv:1108.6047.
 - [13] S. Will, et. al., Nature **465**, 197 (2010).

- [14] O. Dutta, et. al., New J. Phys. **13**, 023019 (2011).
 [15] T. Sowiński, et. al., Phys. Rev. Lett. **108**, 115301 (2012)
 [16] S. Kotochigova and E. Tiesinga, Phys. Rev. A **73**, 041405 (2006).
 [17] M. Yu. Kagan, K. I. Kugel, and D. I. Khomskii, JETP **93**, 415 (2001).
 [18] D.I. Khomskii, Preprint of the P.N. Lebedev Physics Institute no. 105 (1969).
 [19] W. Kohn, and J. M. Luttinger, Phys. Rev. Lett. **15**, 524 (1965).

Supplementary Material for *Orbital physics of polar Fermi molecules*

DERIVATION OF THE PARAMETERS $U_{s,pz}$, $T_{pz,pz}^s$ AND $T_{pz,pxz}^s$

In this section we represent the on-site interaction term $U_{s,pz}$ and interaction-induced hopping terms $T_{pz,pz}^s$ and $T_{pz,pxz}^s$ in terms of the single-particle wavefunction $\mathcal{W}_{i\sigma}(\mathbf{r})$ in orbital σ localized on site \mathbf{i} . Orbital index $\sigma = \{pml\}$ denoting p , m and l levels in x , y , and z direction respectively. Then the s orbitals can be written as $\mathcal{W}_{is}(\mathbf{r}) = w_{ix0}(x)w_{iy0}(y)\phi_0(z)$ where $w_{ix0}(x), w_{iy0}(y)$ are the lowest band Wannier functions and $\phi_0(z)$ is the lowest orbital of the harmonic oscillator in the z direction. Similarly we can write $\mathcal{W}_{ipz}(\mathbf{r}) = w_{ix0}(x)w_{iy0}(y)\phi_1(z)$ and $\mathcal{W}_{ipxz}(\mathbf{r}) = w_{ix1}(x)w_{iy0}(y)\phi_1(z)$. Here $w_{ix1}(x)$ is the Wannier functions in the first band and $\phi_1(z)$ is the first excited state of the harmonic oscillator in the z direction. For simplicity we took $\mathbf{j} = \mathbf{i} + \mathbf{e}_x$. From this we can write various parameters as,

$$U_{s,pz} = \int \{w_{ix0}(x)w_{iy0}(y)\}^2 \{w_{ix0}(x')w_{iy0}(y')\}^2 \Phi_{1,0}(z, z') \mathcal{V}(\mathbf{r} - \mathbf{r}') d\mathbf{r} d\mathbf{r}' \quad (\text{S1a})$$

$$T_{pz,pz}^s(\mathbf{e}_x) = \int w_{jx0}(x)w_{ix0}(x)w_{ix0}^2(x') \{w_{iy0}(y)w_{iy0}(y')\}^2 \Phi_{1,0}(z, z') \mathcal{V}(\mathbf{r} - \mathbf{r}') d\mathbf{r} d\mathbf{r}' \quad (\text{S1b})$$

$$T_{pz,pxz}^s(\mathbf{e}_x) = \int w_{jx1}(x)w_{ix0}(x)w_{ix0}^2(x') \{w_{iy0}(y)w_{iy0}(y')\}^2 \Phi_{1,0}(z, z') \mathcal{V}(\mathbf{r} - \mathbf{r}') d\mathbf{r} d\mathbf{r}' \quad (\text{S1c})$$

$$\Phi_{1,0}(z, z') = \{\phi^1(z)\}^2 \{\phi^0(z')\}^2 - \phi^1(z)\phi^0(z)\phi^1(z')\phi^0(z'). \quad (\text{S1d})$$

The integrations over z, z' can be done analytically using convolution theorem in the momentum space. Consequently in the momentum space we get

$$V(\mathbf{k}_\perp) = \mathcal{F} \left\{ \int \Phi_{1,0}(z, z') \mathcal{V}(\mathbf{r} - \mathbf{r}') dz dz' \right\} = \frac{2\sqrt{2\pi}D^2}{l_z} \left[(kd)^2 - \sqrt{\frac{\pi}{2}} kd(1 + (kd)^2) \text{erfcx} \left(\frac{kd}{\sqrt{2}} \right) \right], \quad (\text{S2})$$

where $\mathcal{F}\{.\}$ denotes Fourier transform, $k = |\mathbf{k}_\perp| = \sqrt{k_x^2 + k_y^2}$, and $l_z = (\hbar/m\Omega)^{1/2}$ is a natural harmonic oscillator length unit. It is important to note that $V(\mathbf{k}_\perp)$ is always negative for any \mathbf{k}_\perp . This explains the appearance of the attractive on-site interaction for any value of the confinement along the z direction. Also we define $\text{erfcx}(x) = \exp(x^2)\text{erfc}(x)$ where $\text{erfc}(\cdot)$ denotes complementary error function.

DERIVATION OF EFFECTIVE INTERACTION IN THE TRIPLET CHANNEL

In this section we derive the p -wave interaction from the Kohn-Luttinger effective interaction in terms of the scattering momentum $\mathbf{q} = \mathbf{k} - \mathbf{k}'$. For this purpose we rewrite Eq. (6) from the original paper

$$V_{\text{eff } s,s}(\mathbf{q}) = V_{\uparrow\uparrow}\eta_{\mathbf{q}} - \sum_{\mathbf{p}} [(V_{\uparrow\uparrow}^2\eta_{\mathbf{q}}^2 + V_{\uparrow\downarrow}^2\beta_{\mathbf{q}}^2) Q_{\mathbf{q},\mathbf{p}} - 2V_{\uparrow\uparrow}^2\eta_{\mathbf{q}}\eta_{\mathbf{k}-\mathbf{p}}Q_{\mathbf{q},\mathbf{p}} - V_{\uparrow\uparrow}^2\eta_{\mathbf{k}'-\mathbf{p}}\eta_{\mathbf{k}-\mathbf{p}}Q_{\mathbf{k}+\mathbf{k}',\mathbf{p}}]. \quad (\text{S3})$$

where $Q_{\mathbf{p},\mathbf{q}} = \frac{f(\epsilon(\mathbf{p})) - f(\epsilon(\mathbf{p}-\mathbf{q}))}{\epsilon(\mathbf{p}-\mathbf{q}) - \epsilon(\mathbf{p})}$ with $f(\cdot)$ being the Fermi distribution function. First we put the expression of $\eta_{\mathbf{q}} = 2(\cos(q_x \tilde{a}) + \cos(q_y \tilde{a}))$ and $\beta_{\mathbf{q}} = 4(\cos(q_x \tilde{a}/2) \cos(q_y \tilde{a}/2))$ back to (S3). As we are interested in p -wave interaction, after expanding (S3) in terms of the momentum k_x, k'_x, k_y, k'_y , we keep terms proportional to $\sin k_x \tilde{a} \sin k'_x \tilde{a} + \sin k_y \tilde{a} \sin k'_y \tilde{a}$. In this way we get

$$\begin{aligned} \{V_{\text{eff}}(\mathbf{q})\} = & \left(2V_{\uparrow\uparrow} - \sum_{\mathbf{p}} Q(\mathbf{q}, \mathbf{p}) [4(V_{\uparrow\downarrow})^2 - 8(V_{\uparrow\uparrow})^2 \{\cos(k_x \tilde{a} - p_x \tilde{a}) + \cos(k_y \tilde{a} - p_y \tilde{a})\}] \right) (\sin k_x \tilde{a} \sin k'_x \tilde{a} + \sin k_y \tilde{a} \sin k'_y \tilde{a}) \\ & + 4(V_{\uparrow\uparrow})^2 \sum_{\mathbf{p}} Q(\mathbf{q}, \mathbf{p}) (\sin k_x \tilde{a} \sin k'_x \tilde{a} \sin^2 p_x \tilde{a} + \sin k_y \tilde{a} \sin k'_y \tilde{a} \sin^2 p_y \tilde{a}) \end{aligned} \quad (\text{S4})$$

where $\mathbf{q} = \mathbf{k} - \mathbf{k}'$. By converting sums to integrals in (S4) we have to compute terms of the form $\int d\mathbf{p} Q(\mathbf{q}, \mathbf{p})$, $\int d\mathbf{p} \sin^2 p_x a_b Q(\mathbf{q}, \mathbf{p})$, and $\int d\mathbf{p} \cos p_x a_b Q(\mathbf{q}, \mathbf{p})$. Function $Q(\mathbf{q}, \mathbf{p})$ is a continuous counterpart of $Q_{\mathbf{q},\mathbf{p}}$. In the limit of vanishing temperature $T \rightarrow 0$ we approximate all integrals $\int d\mathbf{p} G(\mathbf{p}) \frac{f(\epsilon(\mathbf{p})) - f(\epsilon(\mathbf{p}-\mathbf{q}))}{\epsilon(\mathbf{p}-\mathbf{q}) - \epsilon(\mathbf{p})} \approx \int N_{\text{eff}}(\epsilon, \mu_p) \delta_\epsilon f d\epsilon$ for arbitrary function $G(\mathbf{p})$. The effective density of states reads $N_{\text{eff}}(\epsilon, \mu_p) = \int d\mathbf{k} G(\mathbf{k}) \delta(\epsilon - \epsilon_{\mathbf{k}})$. We see that the only first term inside the third bracket in (S4) is not dressed by $\cos(p_x \tilde{a})$ or $\sin(p_x \tilde{a})$. Hence the effective density of states for this term contains Van-Hove singularity. All other terms with in (S4), due to the dressing by $\cos(p_x \tilde{a})$ or $\sin(p_x \tilde{a})$, are analytic. For convenience, we re-express $\{V_{\text{eff}}(\mathbf{q})\}_- = -\lambda(T, \mu) (\sin(k_x \tilde{a}) \sin(k'_x \tilde{a}) + \sin(k_y \tilde{a}) \sin(k'_y \tilde{a}))$, where $\lambda(T, \mu) = 2V_{\uparrow\uparrow} + \frac{V_{\uparrow\uparrow}^2}{\pi T_{\text{eff}}} F_1(T, \mu) - \frac{V_{\uparrow\uparrow}^2}{\pi T_{\text{eff}}} F_2(T, \mu)$. The functions F_1 and F_2 are given by

$$F_1 = \frac{4}{\pi} F \left(1 - (T + |\mu|)^2 / (4T_{\text{eff}}^{\parallel})^2 \right) \quad (\text{S5a})$$

$$F_2 = \frac{2}{\pi} K \left([1 - (T + |\mu|)^2 / (4T_{\text{eff}}^{\parallel})^2] \right), \quad (\text{S5b})$$

where $F(x) = E(x) - (1-x)K(x)$ with $K(\cdot)$ being the Elliptic integral of the first kind and $E(\cdot)$ is the Elliptic integral of the second kind. Then we can write the BCS equation for the transition temperature T_c as [1]

$$V_p N_{\text{eff}}(0, \mu) \log \left| \left(1 - \left[\frac{\mu}{4T_{\text{eff}}^{\parallel}} \right]^2 \right)^{1/2} \frac{4T_{\text{eff}}^{\parallel}}{T_c} \right| = 1, \quad (\text{S6})$$

where the effective density of state is given by $N_{\text{eff}}(\epsilon, \mu) = \sum_{\mathbf{k}} \delta(\epsilon + \mu - \epsilon_{\mathbf{k}}) \sin^2(k_x a_b) \approx F \left(1 - (\epsilon + |\mu|)^2 / (4T_{\text{eff}}^{\parallel})^2 \right) / \pi^2 T_{\text{eff}}^{\parallel}$.

[1] R. Micnas, J. Ranninger, S. Robaszkiewicz, Rev. Mod. Phys. **62**, 113 (1990).